CALIFORNIA STATE SCIENCE FAIR
2009 PROJECT SUMMARY

Name(s)
Y. Symphony Yu

Project Number
S0430

Project Title
The Rotational Barrier of 6-Methylnicotinamide

Abstract

Objectives/Goals
The objective of my project was to determine the rotational barrier of the molecule 6-methylnicotinamide in its liquid state. In accordance with the calculated value, the experimental value of the rotational barrier should be 16.012 ± 0.212 kcal/mol.

Methods/Materials
Methods in proton nuclear magnetic resonance spectroscopy and computational chemistry were implemented to find the rotational barrier. The 6-methylnicotinamide sample, prepared in a solution of deuterated nitrobenzene, is first analyzed using NMR spectroscopy, with data points collected at incremented temperatures. The raw data collected by the Bruker TOPSPIN program is then transferred to Mathematica 7.0 for nonlinear regression. A composite curve is then obtained and the values of enthalpy and entropy solved for.

Results
According to the experiment, the rotational barrier of the molecule 6-methylnicotinamide is 12.6 kcal/mol.

Conclusions/Discussion
The results from the experiment yielded a percent error of 27.079% for the rotational barrier. This large percent error shows some unexpected/unknown sources of error. Because of the large discrepancy between the theoretical and experimental values for the rotational barrier, the results of this experiment are inconclusive, and further experimentation will be required.

Summary Statement
In my project, I determined the rotational barrier of the molecule 6-methylnicotinamide through the use of proton NMR spectroscopy and the implementation of methods in computational chemistry.

Help Received
Used lab equipment at the University of California, Riverside under the supervision of Professor Mueller and graduate students Jin Feng Lai and Ye Tian; Parents helped with putting together the display board.